The Dow Chemical Company
Midland, Michigan 48674

2020 DOW CENTER
December 18, 2001

Ms. Christine Todd Whitman
Administrator
U.S. Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Dear Ms. Whitman:

CHEMICAL RIGHT TO KNOW – HPV CHALLENGE PROGRAM

On behalf of The Dow Chemical Company, I am pleased to submit the robust summaries in IUCLID format for Chloroacetyl Chloride (Cas No.: 79-04-9). As requested, the test plan has been posted onto the U.S. HPV Chemical Tracking System. All documents are in Adobe Acrobat (pdf) files.

We understand this information will be posted on the internet for comments for a period of 120 days. Please forward comments to me at the following address:

Ms. Connie L. Deford
The Dow Chemical Company
2020 Dow Center
Midland, MI 48674

Sincerely,

Connie L. Deford
Global Environment, Health & Safety Manager
(989) 636-6978

AR201-13405A

HIGH PRODUCTION VOLUME (HPV)

CHEMICAL CHALLENGE PROGRAM

TEST PLAN

For

CHLOROACETYL CHLORIDE

Prepared by:

The Dow Chemical Company

December, 2001

EXECUTIVE SUMMARY

The Dow Chemical Company hereby submits for review and public comment the test plan for chloroacetyl chloride (CAC), which we have classified as a closed-system intermediate, under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. It is the intent of The Dow Chemical Company to use existing data and scientific judgment and analyses to adequately characterize the SIDS (Screening Information Data Set) human health, environmental fate and effects, and physicochemical endpoints for this chemical.

Please note that we are aware that there is another producer and an importer of CAC in the United States. We have been in contact with each of these companies to determine if they were interested in joining with Dow in our commitment to the HPV Chemical Challenge Program. Unfortunately, each of these companies declined our invitation to participate with us in making this HPV commitment. Further, we asked them to assess whether their production, handling, and use of CAC would fulfill the criteria outlined by EPA for a closed-system intermediate. Both of these companies confirmed that their production, handling and use of CAC satisfied the Agency's criteria for a closed-system intermediate.

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TEST PLAN FOR CHLOROACETYL CHLORIDE

I. INTRODUCTION

The Dow Chemical Company has voluntarily committed to develop and/or summarize screening level human health effects, environmental effects and fate, and physicochemical test data for chloroacetyl chloride under the Environmental Protection Agency's (EPA's) High Production Volume (HPV) Challenge Program.

This plan identifies the chemical and its CAS number, identifies existing data of adequate quality for the chemical, and provides justification for why additional data does not need to be generated for the chemical under the Program.

II. DESCRIPTION OF CHLOROACETYL CHLORIDE

A. The Chemical

Chloroacetyl chloride (CAC) (CAS No. 79-04-9), a compound manufactured from vinylidene chloride, is used as an intermediate, primarily in the production of agricultural and pharmaceutical compounds. It is a colorless or slightly yellow liquid at room temperature. It has a strong, pungent odor similar to that of hydrochloric acid, which serves as a fairly reliable warning of its presence. However, even at increasing concentrations, the vapors can dull the sense of smell and make detection difficult.

Table 1. Chemical/physical properties Chloroacetyl Chloride

Chemical Abstract Number	79-04-9
Molecular formula	***$CH_2ClOCCl$***
Molecular weight	***112.9***
Physical State	***Colorless to Light yellow liquid***
Freezing Point	**-7.8°F/-22°C**
Boiling point	**223°F/106°F**
Vapor pressure	**33.3 hPa @ 25°C**
Water Solubility	**Reacts to decompose**
Specific Gravity	**1.41 (25/25°C)**

The health hazards to humans can be summarized as follows:
Eyes: Liquid CAC and its vapors may irritate or damage the cornea, causing permanently impaired vision or blindness.
Skin: A single exposure of a few minutes can cause severe burns and may result in rapid absorption of lethal amounts.
Ingestion: There is little likelihood that ingestion will occur in routine industrial

applications. Nevertheless, small amounts may cause burns of the mouth and throat. Ingestion of large amounts can be fatal.
Inhalation: Excessive exposure to vapors may irritate upper respiratory tract, nasal passages and lungs. Pre-existing lung conditions may be aggravated.

There are a limited number of environmental toxicity and fate studies that exist for the chemical itself due to the reactivity of CAC with water. However, since the material hydrolyzes **within minutes** in water to form hydrochloric acid and chloroacetic acid, the material is believed to be analagous to chloroacetic acid, particularly in terms of its environmental effects. Therefore, many of the environmental studies referenced pertain to chloroacetic acid, and are referenced as such below and in the attached Robust Summaries.

III. TEST PLAN RATIONALE

A. Classification of the Chemical as a Closed-System Intermediate

1. Requirements

Classification of chloroacetyl chloride as a closed-system intermediate under the EPA HPV program is dependent upon a number of criteria outlined by EPA. The Dow Chemical Company asserts that chloroacetyl chloride should be regarded as a closed-system intermediate, based on satisfaction of these criteria. In the following paragraphs, information is provided on the extremely limited potential for exposure during manufacturing, transport, and processing.

2. Satisfaction of Requirements

a. Review of Manufacture / Transport / Consumption:
Chloroacetyl Chloride (CAC) is produced in a single facility within The Dow Chemical Company's Michigan Operations Site located in Midland, Michigan. It has been manufactured since 1972. CAC is manufactured in a closed system from vinylidene chloride. The majority of the CAC is consumed within the same facility in the production of other chlorinated derivatives. A very small percentage is sold to off-site customers, who also utilize CAC as an intermediate. After the CAC is produced, it is placed in one of several storage tanks, which are all vented to a scrubber, and located in a dike area. For internal consumption, CAC is transferred to the reactors as needed via pipeline. For off-site consumption, the CAC is loaded, via a closed system with a vapor return line, into isocontainers. The isocontainers are specially designed tanks surrounded by a frame that allow greater portability and also minimizes the potential for damage to occur during transit. The isocontainers are equipped with dry-disconnect fittings, which minimize any potential for leaks to occur during off-loading. The customers, who utilize the CAC, also have vapor recovery systems in place. The storage tank is vented to either a scrubber or back to the bulk container. To ensure a clean disconnect of the line, procedures are in place to purge the unloading line clear of product.

Our off-site customers are very experience in the handling of this material as evidenced by our on-site customer audits. These audits, conducted by our product steward, are required by our Global Product Stewardship Plan to be conducted at least every three years. Dow only approves customers who agree to specific storage and handling recommendations as well as on-site audits.

b. Environmental Fate

The potential for environmental exposure to CAC is negligible. There are minimal releases to the air, which occur through both point source and fugitive releases, but these represent only a fraction (<500 lbs.) of the CAC produced. There have been and should not be any releases to water or land unless a major plant upset occurred. In case of a plant upset or storage tank leak, CAC would be contained in the dike that surrounds the manufacturing and storage area

Since the CAC is consumed entirely as an intermediate, the downstream processing/use will result in yet a smaller fraction of air emissions than described above during manufacturing. As the residual level of CAC in downstream products is typically non-detectable (L.O.D. – 1ppm) and the downstream products are converted into other products, there is essentially no potential for environmental exposure through its use.

c. Human Exposure

The potential for human exposure is also extremely low. The total number of workers within our facility and our customers is less than 30 as the plants producing and processing these materials are small. Due to the very corrosive nature of CAC, personal protective equipment is worn during production, maintenance, distribution, and processing to ensure no personal contact. During normal operation this would include goggles and hard hats. During an operation, such as a line opening, where there is potential for residual CAC to be present, the protective equipment would include goggles, face shield, hard hat, protective full rubber suit, boots and a full-face respirator. Suitable positive-pressure self-contained breathing apparatus would be used for longer-term exposure in emergency situations such as a spill clean up.

Available monitoring data from the production of CAC, which is conducted periodically, indicates that the exposures are well below the industrial hygiene guideline established for CAC. The 8-hour Time-Weighted Average exposure limit for CAC, established by the American Council of Government Industrial Hygienists (ACGIH), is 0.01ppm, Skin, with an Excursion Exposure Limit of 0.05ppm, Skin. A summary of the actual monitoring data, from the activities, which are expected to have the greatest potential for worker exposures, is included in the table on the following page. During these activities, personal protective equipment is worn.

RESULTS FROM CAC INDUSTRIAL HYGIENE MONITORING

ACTIVITY	MONITORING DATA	SAMPLE DURATION	COMMENT
Connecting Loading Hose to CAC Isocontainer	0.005	11 min.	Personal Sample
Disconnecting Loading Hose from CAC Isocontainer	0.03 ppm	15 min.	Personal Sample
Disconnecting Loading Hose from CAC Isocontainer	0.01 ppm	15 min.	Personal Sample

As the residual level of CAC in downstream products is non-detectable (L.O.D. – 1ppm) and the downstream products are converted into other products, there is essentially no potential for worker or public exposure. The only potential for public exposure would be as a result of a significant manufacturing plant upset or transportation incident. We have a program in place to conduct root cause investigations if any such incidents were to occur and to develop a corrective action plan to prevent reoccurrence.

3. Conclusion

The Dow Chemical Company believes that the information above fully satisfies the EPA's criteria for closed-system intermediates. Further, the above information suggests that there appears to be little additional action that could be taken to prevent any further exposure, as the potential exposure opportunity is extremely limited.

B. Human Health Effects

There are six mammalian toxicity endpoints in the HPV Program (Results summarized in table on Page 8):

- Acute Toxicity
- Repeated Dose Toxicity
- Genetic Toxicity *In Vitro*
- Genetic Toxicity *In Vivo*
- Reproductive Toxicity
- Developmental Toxicity

Published and unpublished data, as detailed in the attached Robust Summaries, satisfy the requirements of Acute, Repeated Dose, and *In Vitro* Genetic Toxicity endpoints. Since in vitro genetic toxicity endpoints are negative, in vivo testing is not required. As CAC satisfies the EPA's criteria as a closed-system intermediate, the only data gap that exists is for a

Developmental Toxicity study. We are not proposing to conduct this study because we believe the corrosive nature of CAC would not allow us to conduct a study at a level that would result in any meaningful results. Further, when you consider the product stewardship precautions that are taken by Dow and our customers to minimize exposure, we don't believe that results from a developmental toxicity study would impact our handling recommendations.

The attached Robust Summaries provide adequate data to characterize the human health effects endpoints under the Program.

C. Ecotoxicity

(Results are summarized in a table on Page 8.)

There are three aquatic toxicity endpoints in the HPV Program:

- Acute Toxicity to Fish
- Acute Toxicity to Aquatic Invertebrates
- Toxicity to Algae (Growth Inhibition)

Published and unpublished data for chloroacetic acid, as detailed in the attached Robust Summaries, satisfies requirements for Acute Toxicity to Fish, Aquatic Invertebrates and Toxicity to Algae.

D. Environmental Fate

(Results are summarized in a table on Page 8.)

Predictive models were used to develop meaningful data for chemicals that are gaseous at relevant environmental temperatures and pressures. The environmental fate data includes:

- Photodegradation
- Stability in Water (Hydrolysis)
- Transport and Distribution (Fugacity)
- Biodegradation

1. Photodegradation

Photodegradation was estimated using models accepted by the EPA [2]. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) [1] is used by The Dow Chemical Company. This program calculates a chemical half-life based on an overall OH reaction rate constant, a 12-hr day, and a given OH concentration. This calculation was performed for chloroacetyl chloride, as detailed in the attached Robust Summaries.

2. Stability in Water (Hydrolysis Testing and Modeling)

Chemicals that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters [3]. Stability in water can be estimated using models accepted by the EPA [2]. This value has been calculated for chloroacetyl chloride, as detailed in the attached Robust Summaries.

3. Chemical Transport and Distribution In The Environment (Fugacity Modeling)

Chloroacetyl chloride is one compound in the series of chlorinated acetyl chlorides. These are acetyl chloride, chloroacetyl chloride, dichloroacetyl chloride, and trichloroacetyl chloride. Chloroacetyl chloride displays reactivity with water that is intermediate between acetyl chloride and dichloroacetyl chloride. Acid chlorides react with water to produce the corresponding carboxylic acid, hydrogen ion, and chloride. The generic reaction of acid chlorides and nucleophiles such as water, alcohols, and amines, is used for the laboratory scale preparation of the corresponding acids, esters, and amides and is referred to as an acylation reaction. These reactions proceed exothermically and generally occur rapidly at room temperature.

Chloroacetyl chloride decomposes rapidly and exothermically upon addition to water. An ampoule containing 3 g of CAC reacted completely in 750 mL of water in two hours, which corresponds to a $t_{1/2} < 30$ minutes. The authors note that the rate of reaction was limited by the rate at which CAC went into solution. When CAC is added in a co-solvent (in 150 mL of acetone) to 600 mL of water the reactions proceeded even more rapidly. In the gas phase, hydrolysis of chloroacetyl chloride and water vapor is slow.

Chloroacetyl chloride is highly reactive in water. Thus, the use of a partitioning model such as the multimedia fugacity model (EQulibrium Concentration model, or EQC) to determine its distribution among air, water, and soil does not yield meaningful results. Both Mackay Level I and Level III models were used to assess the fate and transport of CAC in the environment. These models use an equilibrium partition constant to scale or calculate mass transfer between two phases, where the constant is defined as the ratio of the equilibrium concentration in the two phases. A chemical, such as CAC, that reacts rapidly in one phase (water) doesn't have a definable concentration in that phase. Therefore a partition constant or mass transfer coefficient that includes the reactive phase can not be defined. Since these models require calculation of a partition constant between the various environmental compartments, they will provide flawed predictions for the fate and transport of highly reactive compounds such as CAC.

4. Biodegradation Testing

Little is known about the biodegradation of CAC in groundwater or soil. However, since this compound rapidly hydrolyzes in water, study of the biodegradation of CAC would have limited relevance to the environment. The major hydrolysis product, chloroacetic acid, has been well studied and passed the "readily biodegradable" 28-day test. Therefore, we suggest that biodegradability of CAC need not be measured in the laboratory. Rather, supplying information/references on the biodegradation of chloroacetic acid in groundwater will provide insight into the fate of CAC in the environment.

Biodegradation values for chloroacetic acid, as detailed in the attached Robust Summaries, were experimentally determined using OECD Guideline 302B, and used for choroacetyl chloride.

E. Physicochemical Properties

(Results are summarized in the "Description of the Chemical" on page 1.)

The physicochemical properties include:

- Melting Point
- Boiling Point
- Vapor Pressure
- Octanol/Water Partition Coefficient

Data for physicochemical properties will be summarized from various resources and detailed in the attached Robust Summaries.

IV. TEST PLAN SUMMARY

For reasons indicated in the above paragraphs, we do not believe additional data needs to be generated. Due to the manner in which the chemical is manufactured, distributed, and processed; the product stewardship measures taken to prevent exposure; and existing human/environmental data; we believe that our workers, the public and the environment are well protected from exposure to CAC. Additionally, due to the corrosivity of this compound, we do not believe that we could conduct a developmental toxicity study at levels that would produce any meaningful results. Finally, we do not believe that generation of any additional toxicity data will impact our product stewardship practices.

Test Plan for Chloroacetyl Chloride

Endpoint	Data Availability	Acceptable (Reliability)	Planned Testing
Acute Toxicity	LD50 = 207 mg/kg (rat) LC50 = 660 pm (rat) LC50 = 2400 ppm (mouse)	Acceptable (1)	None
Repeated Dose Toxicity	LOAEL = 0.5ppm (rats, mice, hamsters); inhalation 5d/wk for 4 weeks	Acceptable (2)	None
Genetic Toxicity *In Vitro*	Ames: Negative	Acceptable (2)	None
Genetic Toxicity *In Vivo*	Not available	Not necessary	None
Reproductive Toxicity	Not available	Not required	None
Developmental Toxicity	Not available	Not necessary	None
Acute Toxicity to Fish	CAC: LC50 = 369 mg/L (Lebistes reticulatus)	Acceptable (2)	None
Acute Toxicity to Aquatic Invertebrates	EC50 = 22-75 mg/L (Daphnia magna)	Acceptable (2)	None
Toxicity to Algae (Growth Inhibition)	CAC: EC50 = 0.028 mg/L (Scenedesmus subspicatus)	Acceptable (2)	None
Photodegradation	Halflife = 450 days (calculated)	Acceptable (2)	None
Stability in Water (Hydrolysis)	Halflife (pH 7) < 30 minutes at 25 deg. Centrigrade (calculated)	Acceptable (2)	None
Transport and Distribution (Fugacity)	Model does not produce meaningful distribution values due to reactivity in water.	Acceptable	None
Biodegradation	100% after 28 days	Acceptable (2)	None

REFERENCES

1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.02. Syracuse Research Corporation, Syracuse, NY, USA.
2. US EPA. 1999. Determining the Adequacy of Existing Data. OPPT, EPA.
3. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

AR201-13405B

IUCLID

Data Set

New Chemical	:	ID: 79-04-9
CAS No.	:	79-04-9
Generic name	:	Chloroacetyl chloride
Producer Related Part		
Company	:	The Dow Chemical Company
Creation date	:	28.11.2000
Substance Related Part		
Company	:	The Dow Chemical Company
Creation date	:	28.11.2000
Memo	:	
Printing date	:	05.12.2001
Revision date	:	
Date of last Update	:	05.12.2001

1.0.1 OECD AND COMPANY INFORMATION

Type	:	
Name	:	The Dow Chemical Company
Partner	:	
Date	:	
Street	:	2020 Dow Center
Town	:	48674 Midland, Michigan
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	

13.12.2000

1.0.2 LOCATION OF PRODUCTION SITE

Name of Plant	:	The Dow Chemical Company's Michigan Operations Site
Street	:	
Town	:	Midland MI
Country	:	United States
Phone	:	989-636-1000
Telefax	:	
Telex	:	
Cedex	:	
Remark	:	Chloroacetyl Chloride (CAC) is produced in a single facility within The Dow Chemical Company's Michigan Operations Site located in Midland, Michigan. CAC is manufactured from vinylidene chloride in a closed system. The majority of the CAC is consumed within the same facility in the production of other chlorinated derivatives. A very small percentage is sold to off-site customers, who also utilizes CAC as an intermediate. Upon completion of production, the CAC is placed in one of several storage tanks, which are all vented to a caustic scrubber. For internal consumption, CAC is transferred to the reactors as needed via pipeline. For off-site consumption, the CAC is loaded, via a closed system with a vapor return line, into isocontainers. The customers, who off-load the CAC, also have vapor recovery systems in place. Further, off-site customers have handled this material safely for quite some time as evidenced by our on-site customer audits. These audits, conducted by our product steward, are required by our Global Product Stewardship Plan to be held at least every three years.

30.08.2001

1.0.3 IDENTITY OF RECIPIENTS

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	% w/w

14.12.2000

1.1.0 DETAILS ON TEMPLATE

1.7 USE PATTERN

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit	**:**	TLV (US)
Limit value	**:**	.05 other: ppm
Short term exposure		
Limit value	**:**	.15 other: ppm
Schedule	**:**	
Frequency	**:**	times
Remark	**:**	This value carries a skin notation. A "skin" notation following the exposure guideline refers to the potential for dermal absorption of the material. It is intended to alert the reader that inhalation may not be the only route of exposure and that measures to minimize dermal exposures should be considered.
Reliability	**:**	(1) valid without restriction
30.08.2001		

Type of limit	**:**	other: DOW IHG
Limit value	**:**	.01 other: ppm
Short term exposure		
Limit value	**:**	.05 other: ppm
Schedule	**:**	
Frequency	**:**	times
Remark	**:**	This value carries a skin notation. A "skin" notation following the exposure guideline refers to the potential for dermal absorption of the material. It is intended to alert the reader that inhalation may not be the only route of exposure and that measures to minimize dermal exposures should be considered.
Reliability	**:**	(1) valid without restriction
30.08.2001		

2.1 MELTING POINT

Value	:	= -21.8 ° C
Sublimation	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Data are for the flake form of the material.
Source	:	The Dow Chemical Company

14.12.2000 (1)

2.2 BOILING POINT

Value	:	= 106 ° C at
Decomposition	:	
Method	:	
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	The Dow Chemical Company

14.12.2000 (1)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= 33.3 hPa at 25° C
Decomposition	:	
Method		
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Source	:	The Dow Chemical Company

14.12.2000 (1)

2.5 PARTITION COEFFICIENT

2.6.1 WATER SOLUBILITY

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	nm
Rel. intensity	:	based on Intensity of Sunlight
Direct photolysis		
Halflife t1/2	:	= 450 day
Degradation	:	% after
Quantum yield	:	
Deg. Product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Deg. Product	:	79-11-8 Acetic acid, chloro-
Source	:	The Dow Chemical Company
Reliability	:	(1) valid without restriction

30.08.2001 (2)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at degree C
t1/2 pH7	:	< 30 minute(s) at 25 degree C
t1/2 pH9	:	at degree C
Deg. Product	:	
Method	:	other
Year	:	
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	The cited article references experiments to determine the heat of hydrolysis of chloroacetyl chloride. It documents that the reaction, chloroacetyl chloride undergoing hydrolysis to produce hydrochloric acid and chloroacetic acid, required 2 hours to reach completion. The assumption can be made that "reach completion" means that >97% of the parent material has hydrolyzed. The corresponds to the completion of greater than 5 t1/2. Back-calculation then produces a t1/2 of less than 30 minutes, which is too short to be meaningful for environmental considerations.
Source	:	The Dow Chemical Company
Reliability	:	(1) valid without restriction

30.08.2001 (3)

3.1.3 STABILITY IN SOIL

3.2 MONITORING DATA

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	other: mathematical modeling

Air (level I)	:	16
Water (level I)	:	84
Soil (level I)	:	0
Biota (level II / III)	:	0
Soil (level II / III)	:	66.7
Method	:	other: Mackay Level I/III fugacity modeling
Year	:	2001
Source	:	The Dow Chemical Company
Test condition	:	Required Input Values for Level I/III Modeling of Chloroacetyl Chloride

Property	Value
Chemical Type	1
Molecular Mass (g/mol)	112.94
Water Solubility (g/m3)	3.99E+5
Vapor Pressure (Pa)	3300
Melting Point (0C)	-22
Estimated Henry's Law Constant (H) (Pa m3/mol) = (J/mol) Kaw	0.934
Air-Water Partition Coefficient Log Kow	3.77E-4
Octanol-Water Partition Coefficient	-0.22
Temperature (0C)	25
Amount of Chemical input to the System (kg)	100,000

Reliability	:	(1) valid without restriction

05.12.2001 (4)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Contact time	:	
Degradation	:	= 100 % after 28 day
Result	:	readily biodegradable
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(1) valid without restriction

30.08.2001

3.6 BOD5, COD OR BOD5/COD RATIO

BOD5		
Method	:	
Year	:	
GLP	:	no data
Concentration	:	related to
BOD5	:	= .36 mgO2/l
COD		

Method	:	
Year	:	
GLP	:	no data
COD	:	= .51 mg/g substance
RATIO BOD5 / COD		
BOD5/COD	:	= .71
Remark	:	Number cited in COD field is actually ThOD.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (1)

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	
Species	:	Lebistes reticulatus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	c = 369
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001

Type	:	
Species	:	Leuciscus idus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	c = 100 - 500
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001

Type	:	
Species	:	Pimephales promelas (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
LC50	:	c = 145 - 164
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	c = 22 - 75
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (1)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	biomass
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= .028
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (5)

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	biomass
Exposure period	:	72 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= .025
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001

Species	:	Scenedesmus subspicatus (Algae)
Endpoint	:	growth rate
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= .07
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (6)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type	:	
Species	:	Pseudomonas putida (Bacteria)
Exposure period	:	3 hour(s)
Unit	:	mg/l
Analytical monitoring	:	
EC50	:	= 750 - 1000
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (7)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species	:	Daphnia magna (Crustacea)
Endpoint	:	reproduction rate
Exposure period	:	21 day
Unit	:	mg/l
Analytical monitoring	:	
NOEC	:	= 32
LCEC	:	= 100
MATC	:	= 56
Remark	:	Because the material hydrolyzes quickly (t1/2<30 min.) to chloroacetic acid and water, data quoted are taken from chloroacetic acid, summarized in IUCLID data sheet for CAS# 79-11-8. See that sheet for complete summary.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (8)

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	
Sex	:	male/female
Number of animals	:	2
Vehicle	:	other: corn oil
Value	:	ca. 1260 - 2500 mg/kg bw
Method	:	other
Year	:	1955
GLP	:	no data
Test substance	:	no data
Method	:	Young adult male and female rats were fasted overnight. They were administered the material as a 10% solution in corn oil at dose levels of 1260 (male) or 2500 (female) mg/kg bw. Animals were observed closely for two weeks, then submitted for pathological examination. All animals which died prior to scheduled necropsy were also submitted for pathological examination. Body weights were recorded on the day of treatment (Study Day 0), and Study Days 1, 8, and 15.
Result	:	Two of two males fed 1260 mg/kg bw died within 2 hours. Two of two females fed 2500 mg/kg bw survived the observation period with no weight loss.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (1)

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	2
Vehicle	:	other: corn oil
Value	:	= 207 mg/kg bw
Method	:	other
Year	:	1969
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Young adult male and female rats were fasted overnight. They were administered the material as a 50% solution in corn oil at dose levels of 126, 158, 200, or 251 mg/kg bw. Animals were observed closely for 9 days, then submitted for pathological examination. All animals which died prior to scheduled necropsy were also submitted for pathological examination. Body weights were recorded on the day of treatment.
Result	:	Survival time was several hours to 2 days with most deaths occurring within 1 day. Toxic signs included increasing weakness, collapse, and death. Survivors at lower dose levels showed normal weight gain in 7 days, while those at higher dose levels showed only slight weight gain. At autopsy for animals which failed to survive the observation period, the lungs and liver were hemorrhagic and there was gastrointestinal inflammation. Surviving animals were sacrificed 9 days after dosing. Macroscopic examination showed areas of lung congestion, slight discoloration of the liver, and slight gastrointestinal inflammation.
Source	:	The Dow Chemical Company

Reliability : (2) valid with restrictions
30.08.2001 (9)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	rat
Strain	:	Fischer 344
Sex	:	male/female
Number of animals	:	6
Vehicle	:	
Exposure time	:	1 hour(s)
Value	:	= 660 ppm
Method	:	EPA OPP 81-3
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The test material was vaporized into stainless steel and glass 112 liter Rochester-type chambers using a j-tube apparatus. Groups of 6 male and 6 female Fischer 344 rats were exposed to concentrations of 32, 208, 522, or 747 ppm for one hour. nominal chamber concentrations during exposure were calculated based on the amount of test material used and the total air passed through the chamber during each exposure period. Chamber atmospheres were sampled and analyzed for test material content by high performance thin layer chromatography. Animals were observed during exposures and for 14 days after exposure. Body weights were collected on test days 1, 2, 4, 8, 11, and 15. A complete gross pathologic examination was conducted on each rat, either at death prior to study termination or at the end of the observation period.
Source	:	The Dow Chemical Company
Reliability	:	(1) valid without restriction

30.08.2001 (1)

Type	:	LC50
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	10
Vehicle	:	other
Exposure time	:	2 hour(s)
Value	:	= 2400 ppm
Method	:	other
Year	:	1959
GLP	:	no data
Test substance	:	no data
Method	:	Groups of 10 mice were exposed for 2 hours to a range of test material concentrations between 0.5 and 30 mg/l. In addition, groups of 10 mice were exposed for 5 minutes to a range of concentrations between 10 and 65 mg/l. The mice were exposed in giant glass bottles with a capacity of 72.7 and 74.1 l, in accordance with the Kravkov method. Mice were examined for signs of toxicity during the exposure period and for 5 days thereafter. Mice were submitted for macroscopic and microscopic pathological examination upon death or at the end of the observation period.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (10)

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	2
Vehicle	:	
Value	:	= 316 - 501 mg/kg bw
Method	:	other
Year	:	1969
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Approximately 24 hours prior to dosing, the hair was removed from the trunk of 2 laboratory white rabbits/sex/dose with electric clippers. The test material was applied at 126, 200, 316, 501, 794, 1260, 200, 5010, or 10,000 mg/kg body weight under plastic strips. Following application the animals were held in wooden stocks for a 24-hour exposure period. The plastic strips were removed and the animals returned to their cages. The animals were observed during and after exposure and weighed at intervals up to two weeks post-application. The animals were submitted for necropsy examination after death or at the end of the observation period.
Result	:	Survival time was 3 hours to 2 days. Toxic signs included reduced appetite for 3 to 5 days in survivors, increasing weakness, dyspnea, collapse, and death. The test material was corrosive, with injury extending well in to the dermis. At autopsy for animals which died prior to the end of the observation period, there was slightly enlarged gall bladder and hemorrhagic lungs and liver. Surviving animals were sacrificed 14 days after dosing. The viscera appeared normal by macroscopic examination.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (9)

Type	:	other: single dose dermal absorption study
Species	:	rabbit
Strain	:	
Sex	:	male
Number of animals	:	1
Vehicle	:	
Value	:	= 100 mg/kg bw
Method	:	other
Year	:	1970
GLP	:	no data
Test substance	:	no data
Method	:	Approximately 24 hours prior to dosing, the hair was removed from the trunk of a laboratory white rabbit with electric clippers. The test material was applied at 100 mg/kg body weight under an impervious cuff held in place with a cloth bandage taped to the hair. Following application the animal was returned to a holding cage and allowed to eat and drink ad libitum. Following a 24-hour exposure period, the cuff was removed and the skin washed with soap and water. The animal was observed during and after exposure and weighed at

intervals up to two weeks post-application. The animal was then submitted for necropsy examination.

Result : Application of 100 mg/kg body weight for 24 hours resulted in slight to moderate necrosis at the application site. The rabbit failed to gain weight over a 2-week observation period.

Source : The Dow Chemical Company

Reliability : (2) valid with restrictions

30.08.2001 (1)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 1
PDII :
Result : corrosive
EC classification :
Method : other
Year : 1970
GLP : no data
Test substance : no data
Method : These data were obtained during the conduct of a dermal absorption study. See Record 1, Acute Dermal Toxicity.
Reliability : (2) valid with restrictions

30.08.2001 (1)

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 3 minute(s)
Number of animals : 1
PDII :
Result : corrosive
EC classification :
Method : other
Year : 1956
GLP : no data
Test substance : no data
Method : Male rabbits were prepared by shaving the hair from the entire abdomen with a straight razor and barber soap. The animal was then rested for several days to allow any abrasions to heal completely and to be sure skin was suitable for use. The material was applied undiluted for 0.5, 1 or 3 minutes to intact sites on the abdomen. Sites were covered with gauze pads and cloth bandages anchored to hair. Sites were inspected and graded when bandages were removed.

Result : Application to an intact site on the abdomen of a rabbit for 0.5 minutes caused very slight redness, very slight swelling, and necrosis. A similar application, left on for 1 minute, caused slight necrosis which, upon healing, left a scar. A similar application, left on for 3 minutes, caused slight redness and moderate necrosis which, upon healing,

left a scar.

Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (1)

Species	:	rabbit
Concentration	:	undiluted
Exposure	:	Occlusive
Exposure time	:	24 hour(s)
Number of animals	:	3
PDII	:	
Result	:	corrosive
EC classification	:	
Method	:	other
Year	:	1969
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The backs of male and female rabbits were clipped. The test material was appled under plastic strips for 24 hours. Observations for irritation were made during exposure and for several days after application. The data were scored according to the Draize method.
Result	:	The average maximum Draize score was 8.0 out of 8.0 within 2 hours of exposure. Mild discomfort was immediately apparent. Within 10 minutes, the animals exhibited great discomfort with protruded eyes and erratic breathing. Within 1 hour, animals showed great discomfort, but no skin changes were apparent. Within 2 hours, the application sites had severe edema and severe erythema extending well beyond the area of exposure. Necrosis was obvious with injury extending well into the dermis. Within 168 hours, no change had occurred in the areas of necrosis except that the edema and erythema gradually disappeared.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (9)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure Time	:	.5 minute(s)
Comment	:	
Number of animals	:	1
Result	:	corrosive
EC classification	:	
Method	:	other
Year	:	1956
GLP	:	no data
Test substance	:	no data
Method	:	Both eyes of a male New Zealand White rabbit were stained with 5% fluorescein dye and examined for evidence of injury or alterations. The rabbit was then allowed to rest for 24 hours before test. Two drops of the material were introduced into the right eye. The eye was washed within 30 seconds for 2 minutes in a flowing stream of tepid water. Two drops of material were introduced in a similar fashion to the left eye, but this

eye was left unwashed.

Immmediately after instillation into each eye, the rabbit was examined for signs of discomfort. Within 2-3 minutes after the unwashed eye was treated, each eye was observed for conjunctival and corneal response. Similar observations were made on both eyes at 1 hour, 24 hours, 48 hours, and 6-8 days post-treatment. Examinations were conducted both with and without fluorescein dye.

Result : Both the washed and unwashed eyes had similar reactions to contact with the test material: slight pain, very severe conjunctival and corneal irritation which had not healed appreciably within one week. Blindness very probable.
Source : The Dow Chemical Company
Reliability : (2) valid with restrictions
30.08.2001 (1)

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure Time : .5 minute(s)
Comment :
Number of animals : 2
Result : corrosive
EC classification :
Method : other
Year : 1969
GLP : no data
Test substance : as prescribed by 1.1 - 1.4
Method : 0.1 ml of the material were introduced into the right eyes of a male and a female rabbit. In one rabbit, the eye was washed with warm isotonic saline within 30 seconds. In the other rabbit, the eye was washed with warm isotonic saline within 5 seconds.

Immmediately after instillation into each eye, and at intervals for several days, the eye was examined for signs of discomfort and irritation. The observations were scored according to the Draize method.

Result : The maximum Draize score in each eye was 110 out of a possible 110. Immediately after instillation, the rabbits exhibited signs of severe discomfort, including pawing at the eye, keeping the eye closed, and squealing. Within 10 minutes, the eyes had moderate erythema, moderate edema, and discharge. The corneas were opaque, the iris invisible. This remained unchanged up to 168 hours, when the test was terminated.
Source : The Dow Chemical Company
Reliability : (2) valid with restrictions
30.08.2001 (9)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Species : rat
Sex : male/female
Strain : Fischer 344

Route of admin.	:	inhalation
Exposure period	:	6 hours/day
Frequency of treatment	:	5 days/week for 4 weeks
Post obs. period	:	None
Doses	:	0, 0.5, 1, 2.5, or 5 ppm
Control group	:	yes, concurrent vehicle
LOAEL	:	= .5 - ppm
Method	:	EPA OPP 82-4
Year	:	1982
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Inhalation exposures to CAC vapor or filtered air (control) were conducted under dynamic airflow conditions in 14.5 cubic foot stainless steel containers. Test material vapor was generated using a vaporization apparatus and mixed with filtered air to achieve the desired concentration. Nominal concentrations were calculated from this mixture. In addition, chamber concentrations were measured at regular intervals using a gas chromatograph/mass spectrometer. Groups of 10 rats, mice, and hamsters/sex were exposed to 0, 0.5, 1, 2.5, or 5 ppm for 6 hours/day, 5 days/week, for 4 weeks. Animals were observed daily during the test period. Body weights were recorded twice weekly. Blood samples were collected from animals which survived the study period, and clinical chemistry determination were conducted. All animals, including those which died prior to study termination, were submitted for gross necropsy examination. For animals which survived to study termination, brian, heart, liver, kidneys, and testes weights were collected. Samples of representative organs and tissues were saved in 10% neutral phosphate-buffered formalin. Tissues from up to half the dose groups were mounted for microscopic examination.
Result	:	Exposure to CAC rsulted in grossly visible effects in the respiratory tract of rats inhaling 2.5 or 5 ppm; histopathologic changes were observed at doses as low as 0.5 ppm. These changes were a chronic response to an irritant, observed throughout the respiratory tract, most apparent and severe in the nasal region, and consisted of inflammation, hypertrophy, hyperplasia, and occasionally squamous metaplasia in the respiratory epithelium of the nasal mucosa. A NOEL was not established.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions Difficulty in analytical method for assessing chamber concentrations led to calculated mean values with large standard deviations. For this reason, dose levels quoted are the mean minimum analytical chamber concentrations.

30.08.2001 (1)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	TA98, TA100, TA1535, TA1537, TA1538
Concentration	:	0.5-500 micrograms/plate
Cycotoxic conc.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	other

Year	:	1976
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Standard methodology first developed by Ames, 1973. Arochlor 1254 was used to stimulate the metabolic activation system, derived from rat liver homogenate.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (1)

Type	:	Yeast gene mutation assay
System of testing	:	Saccharomyces cerevisiae
Concentration	:	0.01, 0.1, 0.2, 0.3, 0.4, 0.5%
Cycotoxic conc.	:	0.4, 0.5%
Metabolic activation	:	with and without
Result	:	negative
Method	:	other
Year	:	1976
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Standard method for the in vitro yeast mitotic recombination assay. Arochlor 1254 was used to stimulate the metabolic activation system, derived from rat liver homogenate.
Source	:	The Dow Chemical Company
Reliability	:	(2) valid with restrictions

30.08.2001 (1)

5.6 GENETIC TOXICITY 'IN VITRO'

5.7 CARCINOGENITY

5.8 TOXICITY TO REPRODUCTION

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Unpublished data, The Dow Chemical Company

(2) Meylan, W. (1997). SRC - AOP for Microsoft Windows, Version 1.84, Atmospheric half-life estimating software.

(3) Pritchard, H. O., and Skinner, H. A. (1950). The heats of hydrolysis of the chloro-substituted acetyl chlorides. J. Chem. Soc. 1950: 272-276.

(4) Use of Level I and Level III Fugacity-Based Environmental Equilibrium Partitioning Models to evaluate the Transport of Chloroacetyl Chloride (CAS No. 79-04-9). Unpublished data, The Dow Chemical Company.

(5) Kuhn and Pattard (1990). Algal tox tests. Water Res. 24: 31-38.

(6) Kuhn and Pattard (1990). Algal tox. tests. Water Res. 24: 31-38.

(7) Gerike and Gode (1990). The biodegradability and inhibitory threshold concentration of some disinfectants. Chemosphere 21: 799-812.

(8) Kuhn, et al. (1989). Results of the harmful effects of water pollutants to Daphnia magna in the 21-day reproduction test. Water Res. 23: 501-510.

(9) Unpublished data, The Monsanto Company

(10) Herzog, S. (1959). Cercetari experimentale asupra toxicitatii clorurii de cloracetil. Igiena. Bucharest 8: 135-144.